

APPROXIMATING THE BALANCED MINIMUM EVOLUTION PROBLEM

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ABSTRACT. We prove a strong inapproximability result for the Balanced Minimum Evolution Problem. Our proof also implies that the problem remains NP-hard even when restricted to metric instances. Furthermore, we give a MST-based 2-approximation algorithm for the problem for such instances.

1. INTRODUCTION

Let $[n] := \{1, \dots, n\}$ be a set of n species. Let (δ_{ij}) be a $n \times n$ symmetric matrix with nonnegative entries and zeroes on the diagonal, where δ_{ij} represents the *dissimilarity* between species i and j . The *Balanced Minimum Evolution Problem* is to find a *cubic tree* T (every internal vertex has degree 3) with n leaves, together with a bijection between the leaves of T and the n species, so that

$$(1) \quad f(T) := \sum_{i \neq j} \delta_{ij} 2^{1-d_{ij}} = \sum_{i < j} \delta_{ij} 2^{2-d_{ij}}$$

is minimized, where d_{ij} denotes the distance between the leaves for species i and j in T . We point out that our objective function is twice the *length* of the tree T , which is the commonly used objective function.

This computational biology problem was introduced by Desper and Gascuel [3], inspired by work of Pauplin [7], and has been studied, e.g., in [1, 2, 4, 5, 8]. Although no hardness proof for the problem has been published, it appears that it was known to be NP-hard since 2004 (Guillemot [6]). To our knowledge, plain NP-hardness is the strongest hardness result known about the problem. In particular, the complexity of the Balanced Minimum Evolution Problem is still open in case the dissimilarities are restricted to be 0/1, or to satisfy the triangle inequality. Furthermore, the problem is not known to be hard to approximate.

First, in Section 2, we start with preliminaries. Then, in Section 3, we prove that the Balanced Minimum Evolution Problem does not admit any interesting approximation algorithm (unless $P = NP$): the problem is NP-hard to approximate to within a c^n -factor for some constant $c > 1$. Finally, in Section 4, we give a simple 2-approximation algorithm for the problem, in case the dissimilarities δ_{ij} satisfy the triangle inequality. By results of the previous section, the problem is NP-hard in this case.

2. PRELIMINARY REMARKS AND OBSERVATIONS

2.1. Kraft's Inequality. Kraft's inequality for a binary tree with n leaves states that

$$(2) \quad \sum_{i \in [n]} 2^{-d_i} \leq 1,$$

where d_i is the distance from the root r to the i th leaf. It is easy to prove that, if the tree is a binary cubic tree (meaning that all internal vertices have degree 3 except the root), then

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equality holds in (2). This implies that for every feasible solution T to the Balanced Minimum Evolution Problem and for every fixed leaf j ,

$$(3) \quad \sum_{\substack{i \in [n] \\ i \neq j}} 2^{2-d_{ij}} = 2.$$

2.2. The Objective as an Average Over Compatible Tours. A result of Semple and Steel [8] states that $2^{2-d_{ij}}$ is the probability that leaves i and j are consecutive in a (undirected) tour on the leaves of T chosen uniformly at random from the tours *compatible* with T , that is, such that the tree T can be embedded in the plane so that the tour visits the leaves of T in clockwise order. Thus, we have the following lemma.

Lemma 2.1. *For all feasible solutions T to the Balanced Minimum Evolution Problem, $f(T)$ is the expected cost of a random tour compatible with T .*

In the light of Lemma 2.1, it should not surprise the reader that one can define the Balanced Minimum Evolution Problem over *all* trees T with n leaves, by defining $f(T)$ as the expected cost of a tour picked uniformly at random from the tours compatible with T . Then, letting $P_{ij} = P_{ij}(T)$ denote the unique $i-j$ path in T (with vertex set $V(P_{ij})$) and

$$(4) \quad \pi_{ij} := 2 \prod_{\substack{u \in V(P_{ij}) \\ u \neq i,j}} \frac{1}{\deg_T(u) - 1},$$

one has

$$f(T) = \sum_{i < j} \delta_{ij} \pi_{ij}.$$

However, it is known that the π -matrices of non-cubic trees are convex combinations of the π -matrices of cubic trees [5], hence for every non-cubic tree T there always exists a cubic tree T' with $f(T') \leq f(T)$. In Section 4, we will give a polynomial time algorithm to find such a cubic tree T' .

2.3. The “All 1” Case. Every solution is optimal in that case:

Lemma 2.2. *Suppose $\delta_{ij} = 1$ for every i, j with $i \neq j$. Then, for all feasible solutions T ,*

$$f(T) = n.$$

In particular, the optimum of the Balanced Minimum Evolution Problem is n .

Proof 1. By (3),

$$f(T) = \sum_{i < j} 2^{2-d_{ij}} = \frac{1}{2} \sum_{j \in [n]} \sum_{\substack{i \in [n] \\ i \neq j}} 2^{2-d_{ij}} = \frac{1}{2} 2n = n$$

□

Proof 2. Every tour on the leaves of T has n edges, of cost 1 each. By Lemma 2.1, it follows that $f(T) = n$ for all feasible solutions T . □

3. NP-HARDNESS AND INAPPROXIMABILITY

Theorem 3.1. *There exists a constant $c > 1$ such that the Balanced Minimum Evolution Problem has no c^n -approximation algorithm unless $P = NP$, where n denotes the number of species. This remains true even when all entries of the dissimilarity matrix are in $\{0, 1\}$.*

Proof. The reduction is from the 3-Colorability Problem: We are given a (simple, undirected) graph G on p vertices, and have to decide whether $V(G)$ can be partitioned into three stable sets (recall that a *stable set* is a set of mutually non-adjacent vertices).

We may assume without loss of generality that G contains two vertex-disjoint triangles. Indeed, if not it suffices to add twice three new vertices to G that form a triangle; this has clearly no influence on whether G is 3-colorable or not.

Let λ be an arbitrary constant with $1/2 < \lambda < 2/3$. We will prove the claim with

$$c := 2^{(2/3-\lambda)(3-4\lambda)} > 1.$$

(By taking λ sufficiently close to $1/2$, one has $c \geq 1.12$.)

Let m be the number of edges in G . We may assume

$$(5) \quad m \leq 2^{(2/3-\lambda)p} = 2^{(2/3-\lambda)|V(G)|}$$

because otherwise G has bounded size and we can check whether G is 3-colorable using brute force.

Define k as the smallest integer satisfying $k \geq p/(2\lambda - 1)$ and $k \equiv 1 \pmod{3}$. Consider an arbitrary ordering v_1, v_2, \dots, v_p of the vertices of G . We define an instance of the Balanced Minimum Evolution Problem with $n := p+k$ species as follows. The first p species are associated with the vertices of G : species i (for $i \in [p]$) corresponds to vertex v_i . The matrix (δ_{ij}) is defined by setting, for $i \neq j$,

$$\delta_{ij} := \begin{cases} 1 & \text{if } i, j \in [p] \text{ and } v_i v_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Consider an optimal solution for the instance of the Balanced Minimum Evolution Problem described above. This solution is a cubic tree T with n leaves together with a bijection from the set of species to the set of leaves of T . For simplicity, we denote by v_i ($i \in [n]$) the leaf of T associated to species i . (Thus, when $i \leq p$, v_i denotes both the i th vertex of G and the corresponding leaf of T ; which one is meant will be clear from the context.) The cost of this optimal solution is denoted OPT . Thus, we have

$$(6) \quad OPT = \sum_{v_i v_j \in E(G)} 2^{2-d_{ij}}$$

where d_{ij} is the distance between species i and j in T .

First we show:

$$(7) \quad \text{If } d_{ij} > \lambda k \text{ for all } v_i v_j \in E(G) \text{ then } G \text{ is 3-colorable.}$$

Consider an arbitrary triangle in G ; without loss of generality we may assume that the vertices of this triangle are v_1, v_2, v_3 . Let C be the union of the v_1-v_2 path, the v_1-v_3 path, and the v_2-v_3 path in T . (Recall that there is unique path between two given vertices in a tree, thus C is well defined.) Then C is isomorphic to a subdivision of the claw $K_{1,3}$ and its three leaves are v_1, v_2 , and v_3 . Let w be the unique vertex in C with degree 3. Let P_ℓ ($\ell \in \{1, 2, 3\}$) denote the path obtained from the $v_\ell-w$ path in T by removing w . Since v_1, v_2, v_3 are pairwise adjacent in G , we have

$$(8) \quad |P_\ell| + |P_{\ell'}| = d_{\ell\ell'} > \lambda k$$

for all $\ell, \ell' \in \{1, 2, 3\}$ with $\ell \neq \ell'$. ($|P_\ell|$ stands for the number of vertices in P_ℓ .)

Let T_ℓ ($\ell \in \{1, 2, 3\}$) be the component of $T - w$ containing v_ℓ , and let X_ℓ be the set of internal vertices in T that are included in T_ℓ . Observe that T has $n - 2$ internal vertices and that all vertices of P_ℓ ($\ell \in \{1, 2, 3\}$) are internal vertices of T , except for v_ℓ . Using (8) and $k \geq p/(2\lambda - 1)$ we obtain

$$(9) \quad |X_\ell| \leq (n - 2) + 1 - \sum_{\ell' \in \{1, 2, 3\}, \ell' \neq \ell} |P_{\ell'}| < n - \lambda k - 1 = (1 - \lambda)k + p - 1 \leq \lambda k - 1$$

for all $\ell \in \{1, 2, 3\}$.

Let S_ℓ ($\ell \in \{1, 2, 3\}$) be the set of vertices v_i of G such that v_i is a leaf of T that is included in T_ℓ . (Thus $S_1 \cup S_2 \cup S_3 = V(G)$.) Every two vertices in S_ℓ are at distance at most $|X_\ell| + 1 < \lambda k$ in T by (9). Therefore, S_1, S_2, S_3 are stable sets of G , and G is 3-colorable. This proves (7).

Next we prove:

- (a) if G is not 3-colorable then $OPT \geq 2^{2-\lambda k}$;
- (b) if G is 3-colorable then $OPT \leq m \cdot 2^{2-(2k+4)/3}$.

The first part of the above claim is a direct consequence of (7): If G is not 3-colorable then there is an edge $v_i v_j$ of G such that $d_{ij} \leq \lambda k$, and hence $OPT \geq 2^{2-d_{ij}} \geq 2^{2-\lambda k}$.

For the second part, let S_1, S_2, S_3 denote the three color classes of a 3-coloring of G . Recall that G has two vertex-disjoint triangles, which implies $|S_\ell| \geq 2$ for every $\ell \in \{1, 2, 3\}$. We build a feasible solution T' from this coloring which will imply the desired upper bound on OPT .

The tree T' is defined as follows. First, for each $\ell \in \{1, 2, 3\}$, create a path P_ℓ on $(k-1)/3 + |S_\ell| - 1$ vertices (here we use that $k \equiv 1 \pmod{3}$). Let a_ℓ and b_ℓ be the two endpoints of P_ℓ . Create a new vertex w and make it adjacent to b_1, b_2 , and b_3 . Next, attach a leaf to each vertex of degree 2 in the resulting tree, and attach two new leaves to each of a_1, a_2 , and a_3 . This defines the tree T' . The species are placed in the following way on the leaves of T' : for each $\ell \in \{1, 2, 3\}$, put the species corresponding to vertices in S_ℓ on the $|S_\ell|$ leaves that are closest to a_ℓ in T' , in an arbitrary way. The remaining k species are placed arbitrarily on the k leaves of T' that remain free.

Since $|S_\ell| \geq 2$ for every $\ell \in \{1, 2, 3\}$, the two leaves adjacent to a_ℓ are associated with species in $[p]$, and thus the first $(k-1)/3$ vertices of the path from b_ℓ to a_ℓ in T' are adjacent to leaves associated with species not in $[p]$. Hence, if $i, j \in [p]$ are species such that $v_i v_j \in E(G)$, then they are at distance at least $(k-1)/3 + 1 + (k-1)/3 + 1 = (2k+4)/3$ in T' . Therefore, the cost of this feasible solution is at most $m \cdot 2^{2-(2k+4)/3}$, implying $OPT \leq m \cdot 2^{2-(2k+4)/3}$ as claimed.

Now, since

$$\begin{aligned} \frac{2^{2-\lambda k}}{m \cdot 2^{2-(2k+4)/3}} &= \frac{2^{(2/3-\lambda)k+4/3}}{m} \\ &> \frac{2^{(2/3-\lambda)k}}{m} \\ &\geq 2^{(2/3-\lambda)(k-p)} && \text{(by (5))} \\ &= 2^{(2/3-\lambda)(n-2p)} \\ &\geq 2^{(2/3-\lambda)(3-4\lambda)n} && \text{(since } p \leq (2\lambda-1)k \leq (2\lambda-1)n\text{)} \\ &= c^n, \end{aligned}$$

it follows that a c^n -approximation algorithm for the Balanced Minimum Evolution Problem could be used to decide whether G is 3-colorable or not. This concludes the proof. \square

An instance of the Balanced Minimum Evolution Problem is said to be *metric* if the dissimilarity matrix (δ_{ij}) is a semimetric, that is, if the δ_{ij} 's satisfy

$$\delta_{ik} \leq \delta_{ij} + \delta_{jk}$$

for all distinct species i, j, k .

Corollary 3.2. *The Balanced Minimum Evolution Problem is NP-hard on metric instances. This remains true even if the non-diagonal entries of the dissimilarity matrix are all in $\{1, 2\}$.*

Proof. By Theorem 3.1 the Balanced Minimum Evolution Problem is NP-hard when all dissimilarities are in $\{0, 1\}$. Consider such an instance and add 1 to every non-diagonal entry of the dissimilarity matrix (δ_{ij}) , giving a dissimilarity matrix (δ'_{ij}) . Then (δ'_{ij}) is a semimetric, because

$$\delta'_{ik} \leq 2 = 1 + 1 \leq \delta'_{ij} + \delta'_{jk}$$

for all distinct species i, j, k .

Consider a feasible solution T to the instance, and let $f(T, (\delta_{ij}))$ and $f(T, (\delta'_{ij}))$ denote the cost of the solution w.r.t. (δ_{ij}) and (δ'_{ij}) , respectively. Let $(u_{ij}) := (\delta'_{ij}) - (\delta_{ij})$. Then $f(T, (\delta'_{ij})) = f(T, (\delta_{ij})) + f(T, (u_{ij})) = f(T, (\delta_{ij})) + n$ by Lemma 2.2. It follows that a solution to the modified instance is optimal if and only if it is optimal for the original instance. \square

4. A 2-APPROXIMATION ALGORITHM FOR METRIC INSTANCES

In this section we assume that the dissimilarity matrix (δ_{ij}) is a semimetric. We describe a MST-based 2-approximation algorithm for this special case.

4.1. Two Lower Bounds. Let TSP denote the cost of an optimal tour on the n species with respect to the costs δ_{ij} , and let again OPT denote the cost of an optimal solution to the Balanced Minimum Evolution Problem. By Lemma 2.1, because the average of a random variable is always at least the minimum value achieved by the random variable, we conclude

$$OPT \geq TSP.$$

Now let MST denote the cost of a minimum spanning tree on the species w.r.t. the costs δ_{ij} . It is known that MST is a lower bound on TSP , thus also

$$(10) \quad OPT \geq MST.$$

Algorithm 1 A 2-approximation algorithm for metric instances.

- 1: Compute a minimum spanning tree T_0 on the n species w.r.t. costs δ_{ij} .
 - 2: $T \leftarrow T_0$
 - 3: **while** there is a species $i \in V(T)$ that is not a leaf **do**
 - 4: Relabel internal vertex i as i' .
 - 5: Add new leaf to T adjacent to i' through a new edge of zero cost, label the leaf i .
 - 6: **end while**
 - 7: Find a feasible cubic tree T' with $f(T') \leq f(T)$.
 - 8: **return** T'
-

4.2. The Algorithm and its Analysis. Consider Algorithm 1 above.

First, it is clear that the cost of T_0 , as a solution of the minimum spanning tree problem, is MST .

Second, observe that the modifications performed on T in steps 3–6 induce an extended semimetric $(\hat{\delta}_{ij})$ defined over the whole vertex set of the final tree T . In this semimetric, for every leaf i that was moved to the exterior of the tree, we have $\hat{\delta}_{ii'} = 0$.

Third, observe that the final tree T is an optimal solution of the minimum spanning tree problem with respect to the extended semimetric $(\hat{\delta}_{ij})$, of cost MST . Hence, every closed walk that visits each edge of T twice has cost $2MST$. Since any tour on the leaves of T that is compatible with T can be obtained by shortcircuiting such a closed walk, every such tour has cost at most $2MST$, because $(\hat{\delta}_{ij})$ is a semimetric.

Fourth, by combining Lemma 2.1 and (10), we conclude that Algorithm 1 returns a feasible solution T' whose cost is at most $2MST$, hence at most $2OPT$. It follows from Lemma 4.1 below that the whole algorithm, and in particular step 7, can be implemented so that its running time is polynomial.

Lemma 4.1. *Let T be any tree with n leaves, namely, the n species. Then one can find in polynomial time a feasible cubic tree T' with $f(T') \leq f(T)$.*

Proof. Pick an internal vertex u with degree $q > 3$. Next, pick two neighbors v_1 and v_2 of u . Let $T^{v_1 v_2}$ denote the tree obtained from T by adding a new internal vertex u' with neighborhood $\{u, v_1, v_2\}$ and deleting v_1 and v_2 from the neighborhood of u . We claim that the π -matrix of T , as defined by (4), can be obtained as a convex combination of the π -matrices of the trees $T^{v_1 v_2}$, where $v_1, v_2 \in N_T(u)$. In particular, there exists a pair v_1, v_2 such that $f(T^{v_1 v_2}) \leq f(T)$. The lemma follows from the claim.

In order to prove the claim, denote by (π_{ij}) the π -matrix of T and by $(\pi_{ij}^{v_1 v_2})$ the π -matrix of $T^{v_1 v_2}$. Consider a pair i, j of leaves of T .

If $u \notin P_{ij}(T)$, then $\pi_{ij}^{v_1 v_2} = \pi_{ij}$ always.

Otherwise, $u \in P_{ij}(T)$. Let n_u , $n_{u'}$, $n_{uu'}$ denote the number of pairs v_1, v_2 such that $P_{ij}(T^{v_1 v_2})$ contains, respectively, u and not u' , u' and not u , both u and u' . Then $n_u = 1$, $n_{uu'} = 2(q - 2)$ and $n_{u'} = \binom{q}{2} - n_u - n_{u'} = \frac{1}{2}q^2 - \frac{5}{2}q + 3$.

Therefore,

$$\begin{aligned}
\sum_{\{v_1, v_2\} \subseteq N(u)} \frac{1}{\binom{q}{2}} \pi_{ij}^{v_1 v_2} &= \frac{1}{\binom{q}{2}} \left(\frac{q-1}{2} n_u + \frac{q-1}{q-2} n_{u'} + \frac{q-1}{2(q-2)} n_{uu'} \right) \pi_{ij} \\
&= \frac{2}{q(q-1)} \left(\frac{q-1}{2} + \frac{q-1}{q-2} \left(\frac{1}{2}q^2 - \frac{5}{2}q + 3 \right) + \frac{q-1}{2(q-2)} 2(q-2) \right) \pi_{ij} \\
&= \frac{2}{q} \left(\frac{1}{2} + \frac{1}{q-2} \left(\frac{1}{2}q^2 - \frac{5}{2}q + 3 \right) + 1 \right) \pi_{ij} \\
&= \frac{2}{q} \frac{1}{q-2} \left(\frac{q-2}{2} + \frac{1}{2}q^2 - \frac{5}{2}q + 3 + q - 2 \right) \pi_{ij} \\
&= \frac{2}{q} \frac{1}{q-2} \left(\frac{1}{2}q^2 - q \right) \pi_{ij} \\
&= \pi_{ij}.
\end{aligned}$$

From what precedes, we infer that

$$\sum_{\{v_1, v_2\} \subseteq N(u)} \frac{1}{\binom{q}{2}} \pi_{ij}^{v_1 v_2} = \pi_{ij}$$

for all pairs of leaves i, j . The claim, and the result follow. \square

Our final result follows.

Theorem 4.2. *Algorithm 1 is a 2-approximation algorithm for the Balanced Minimum Evolution Problem.*

4.3. Tightness of the Lower Bounds. Consider the metric instances of the Balanced Minimum Evolution Problem with $\delta_{1i} = 1$ for all $i > 1$ and $\delta_{ij} = 2$ for all pairs such that $i > 1$ and $j > 1$. For these instances, $MST = n - 1$. However, as it can be easily checked, we also have $OPT \geq 2n - 2$. Hence, $\lim_{n \rightarrow \infty} \frac{OPT}{MST} = 2$ for this family of instances. This indicates that analyzing the approximation factor of an algorithm in terms of MST cannot yield a factor smaller than 2.

We believe that this is even true when the stronger bound TSP is used, and make the following conjecture (backed by experimental evidence).

Conjecture 4.3. *The family of instances of the Balanced Minimum Evolution Problem in which (δ_{ij}) is the shortest path metric of a n -vertex cycle satisfies $\lim_{n \rightarrow \infty} \frac{OPT}{TSP} = 2$.*

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